Supplementary Information Document for

"Influence of sample momentum space features on scanning tunnelling microscope measurements"

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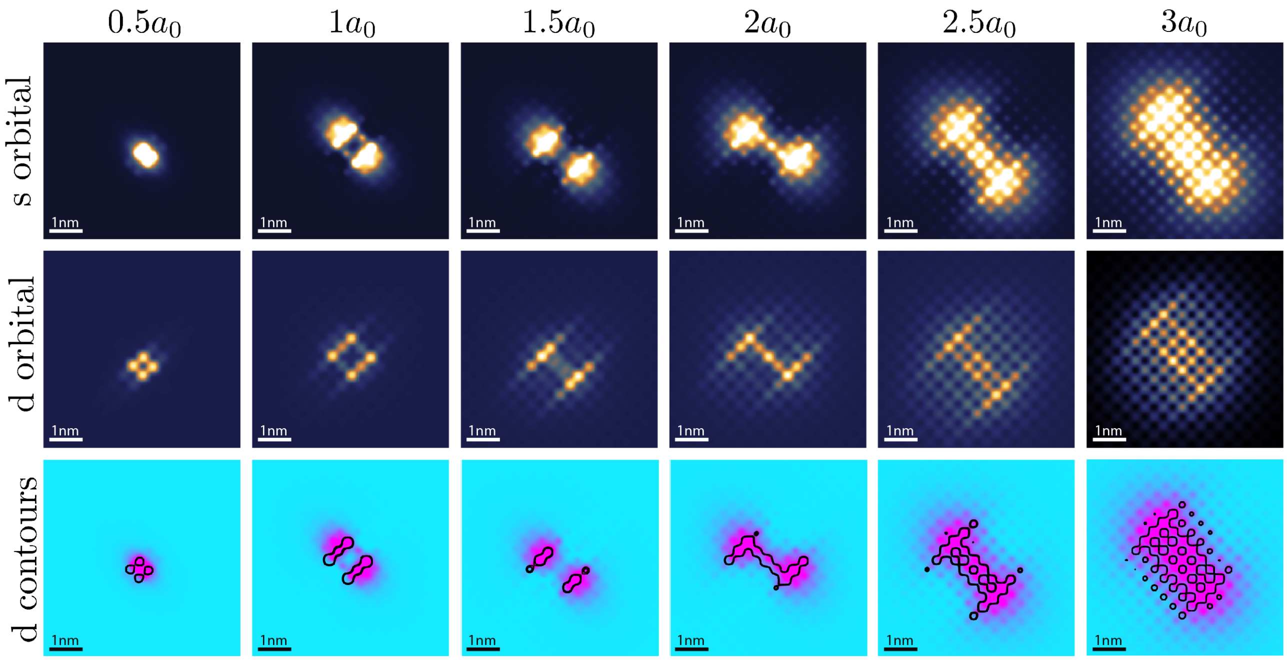
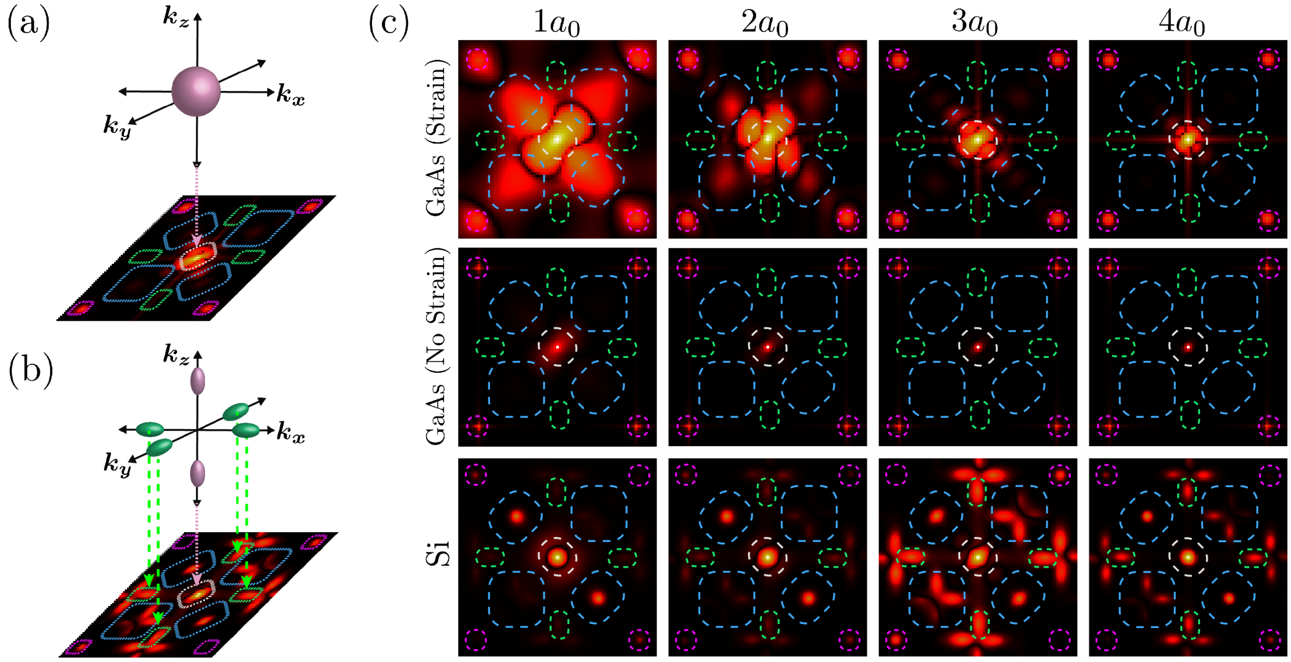
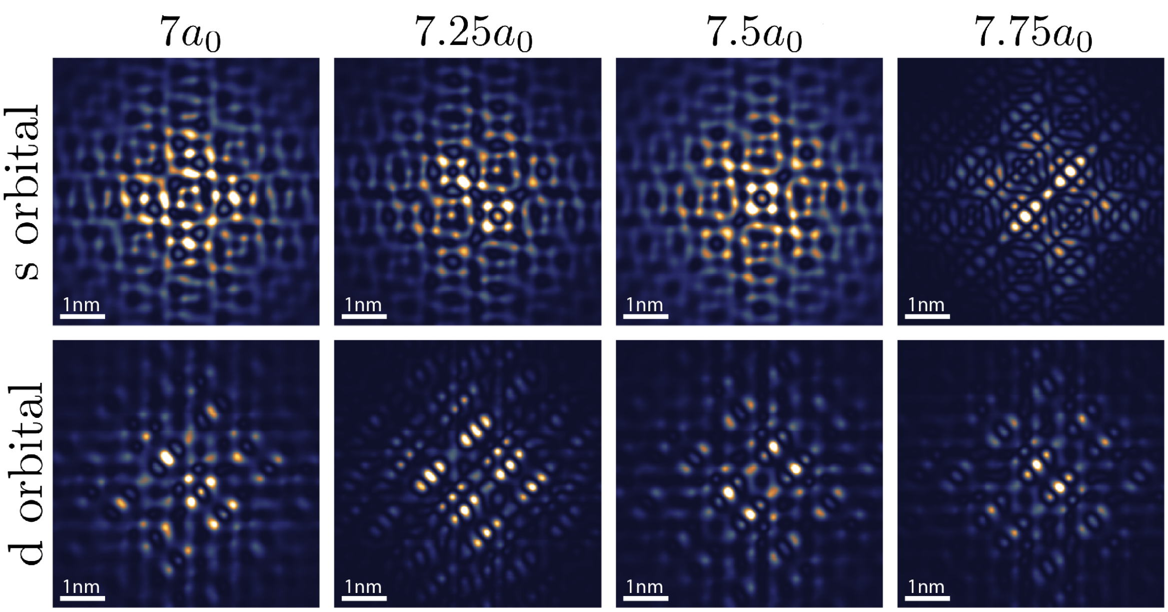


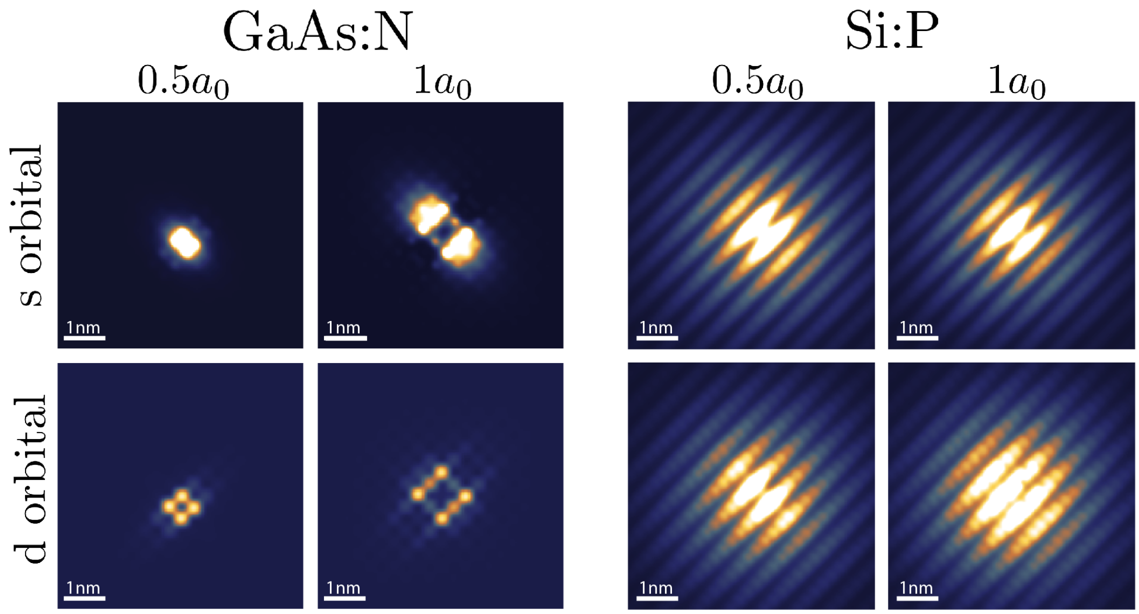
Supplementary Fig. S1. STM images of N impurities in GaAs for each of the first 6 planes, both *s* (top row) and *d* (middle row) images. Gaussian blurring and colour saturation has been applied to the images which is commensurate with the experimental observations. The contours of the *d* images overlaid on top of the *s* images (bottom row) which show a good agreement between the two sets of images.



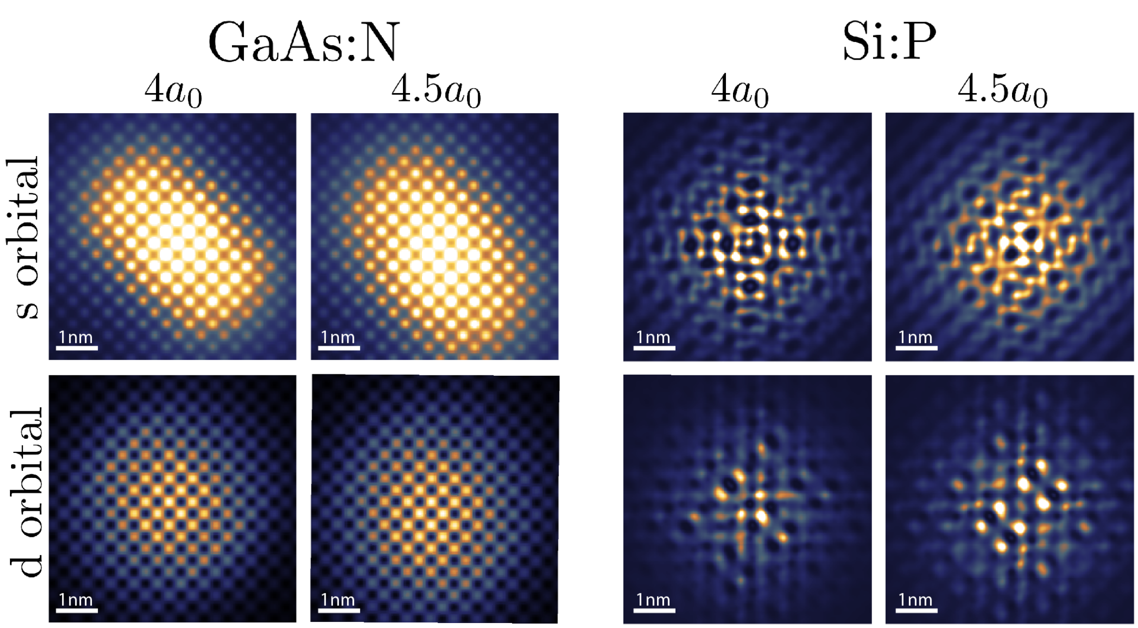
Supplementary Fig. S2. (a) Schematic plot indicating the projection of 3-dimensional valley space on 2-dimensional STM image Fourier spectra for a direct bandgap material such as GaAs:N studied in this work. (b) Schematic plot indicating the projection of 3-dimensional valley space on 2-dimensional STM image Fourier spectra for an indirect bandgap material such as Si:P studied in this work. (c) Fourier transforms of STM images of impurity wave functions. Beyond a few layers from the surface the N impurity states have simpler Fourier spectra, consisting only of low frequency components and periodic components at the reciprocal lattice vectors. The features which occur in the highlighted blue regions in the GaAs:N Fourier spectra are attributed to the lattice strain around the N impurity atom, as they disappear when the strain is artificially turned off and N impurity is placed in unperturbed GaAs lattice. The Fourier spectra of the P donors are more involved. The highlighted features in the Si:P spectra reflect: the low frequency probability envelope and z valleys projection (white), the x and y valleys (green), $2\times$ 1 surface reconstruction induced features (blue), and the periodic components (pink). As expected from the valley re-population effect, shallow Si:P systems exhibit almost no features in the green regions indicating that x and y valleys are now de-populated.



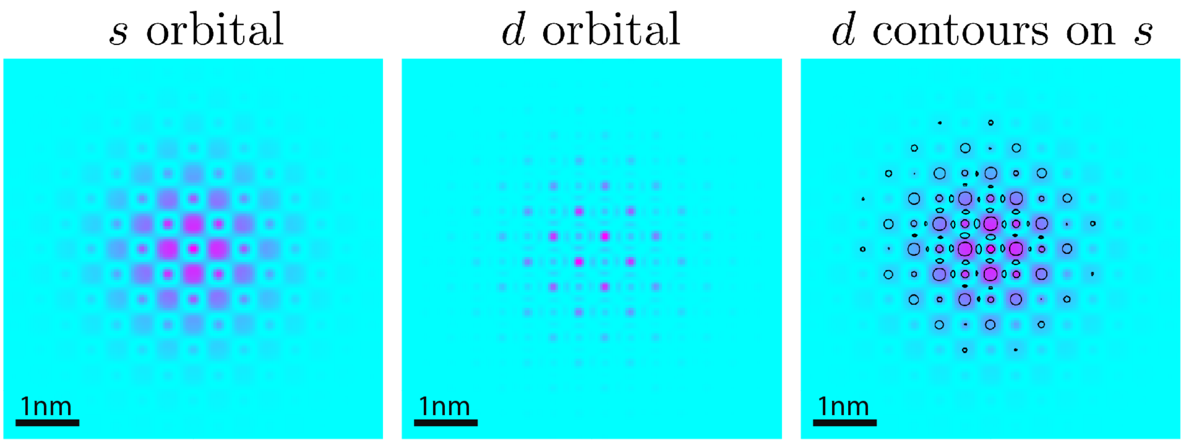
Supplementary Fig. S3. The computed STM images of deeper P impurities in Si are shown for both x and d tip orbitals. At these deeper depths the emergence of the full valley structure results in complicated image feature maps, which makes s and d orbital images distinctly different.



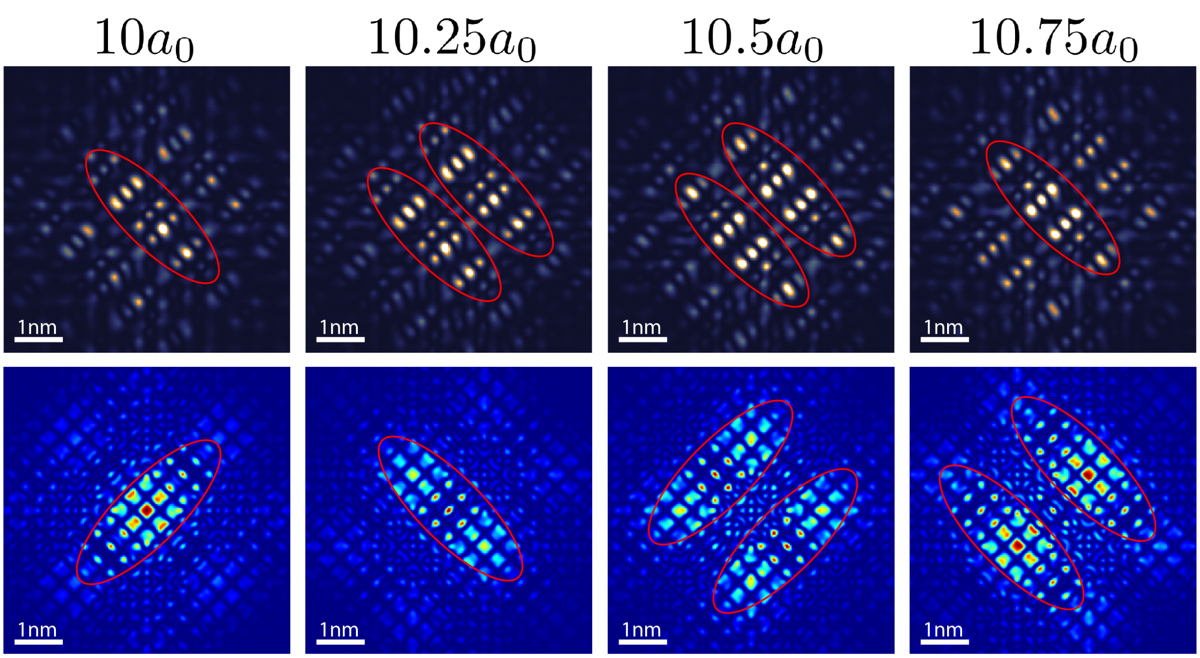
Supplementary Fig. S4. The computed STM images of GaAs:N and Si:P systems are plotted for a few shallow depths of N and P impurities. In both cases, the s and d images are qualitatively similar. For Si:P case, the similarity of s and d orbital images is due to significant valley re-population effect at shallow donor depths which leads to donor wave functions comprised of dominantly z valleys. The absence of x and y valleys lead to disappearance of complex image feature maps typically observed at deeper depths.



Supplementary Fig. S5. The computed STM images of GaAs:N and Si:P for a few selected deep depths. While in the case of GaAs:N the s and d images are qualitatively similar, for Si:P drastic differences is observed between s and d cases.



Supplementary Fig. S6. The s and d images resulting from a typical Kohn-Luttinger based simulation with the valleys removed. By overlaying the contours of the d image on top of the corresponding s image, we find that almost all features are in direct correspondence, with the main difference being a broadening of the features of the s image. As experimental measurements typically exhibit broadened features due to inherent blurring caused by noise, such qualitative differences will be hard to distinguish in measured images.



Supplementary Fig. S7. The tight-binding and corresponding Kohn-Luttinger (KL) images for a few selected deep donor depths. The images show qualitatively the repeating "butterfly and caterpillar" structures in both cases. The KL images display alternating symmetry axes, as earlier reported in Ref. [35].